



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:29 AM UTC

PDB ID : 9YWN / pdb_00009ywn
Title : Protein Structure of the First Glycoside Hydrolase Family 30, Subfamily 12
Endoxylanase
Authors : St John, F.J.; Tan, K.
Deposited on : 2025-10-24
Resolution : 1.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

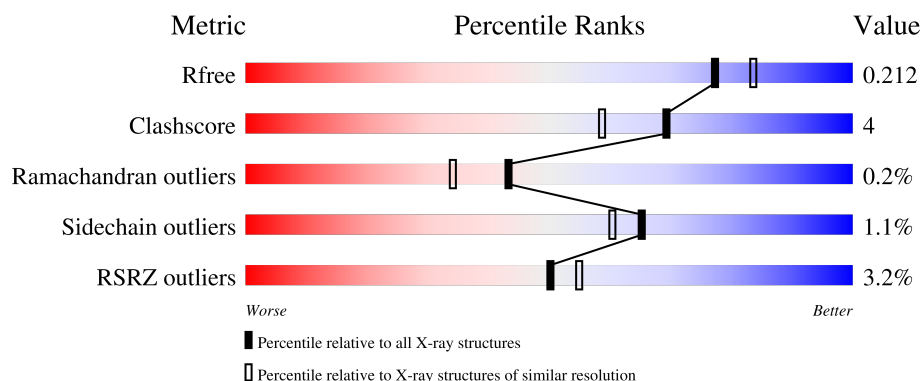
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	447	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	447	<div> <div>0%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	C	447	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> </div>
1	D	447	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>5%</div> </div> </div>
1	E	447	<div> <div>8%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	447	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	E	502	-	-	X	-
2	GOL	E	506	-	-	X	-
4	ACY	C	507	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22256 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glucuronoarabinoxylan endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	10	0
			3391	2166	551	664	10			
1	B	424	Total	C	N	O	S	0	10	0
			3394	2166	551	667	10			
1	C	424	Total	C	N	O	S	0	10	0
			3387	2163	549	665	10			
1	D	424	Total	C	N	O	S	0	12	0
			3404	2174	553	667	10			
1	E	424	Total	C	N	O	S	0	9	0
			3388	2163	550	665	10			
1	F	424	Total	C	N	O	S	0	7	0
			3383	2159	551	663	10			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP A0A369AIV8
A	-23	HIS	-	expression tag	UNP A0A369AIV8
A	-22	HIS	-	expression tag	UNP A0A369AIV8
A	-21	HIS	-	expression tag	UNP A0A369AIV8
A	-20	HIS	-	expression tag	UNP A0A369AIV8
A	-19	HIS	-	expression tag	UNP A0A369AIV8
A	-18	HIS	-	expression tag	UNP A0A369AIV8
A	-17	SER	-	expression tag	UNP A0A369AIV8
A	-16	SER	-	expression tag	UNP A0A369AIV8
A	-15	GLY	-	expression tag	UNP A0A369AIV8
A	-14	VAL	-	expression tag	UNP A0A369AIV8
A	-13	ASP	-	expression tag	UNP A0A369AIV8
A	-12	LEU	-	expression tag	UNP A0A369AIV8
A	-11	GLY	-	expression tag	UNP A0A369AIV8
A	-10	THR	-	expression tag	UNP A0A369AIV8
A	-9	GLU	-	expression tag	UNP A0A369AIV8
A	-8	ASN	-	expression tag	UNP A0A369AIV8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	expression tag	UNP A0A369AIV8
A	-6	TYR	-	expression tag	UNP A0A369AIV8
A	-5	PHE	-	expression tag	UNP A0A369AIV8
A	-4	GLN	-	expression tag	UNP A0A369AIV8
A	-3	SER	-	expression tag	UNP A0A369AIV8
A	-2	ASN	-	expression tag	UNP A0A369AIV8
A	-1	ALA	-	expression tag	UNP A0A369AIV8
A	0	MET	-	expression tag	UNP A0A369AIV8
A	422	GLU	-	cloning artifact	UNP A0A369AIV8
B	-24	MET	-	initiating methionine	UNP A0A369AIV8
B	-23	HIS	-	expression tag	UNP A0A369AIV8
B	-22	HIS	-	expression tag	UNP A0A369AIV8
B	-21	HIS	-	expression tag	UNP A0A369AIV8
B	-20	HIS	-	expression tag	UNP A0A369AIV8
B	-19	HIS	-	expression tag	UNP A0A369AIV8
B	-18	HIS	-	expression tag	UNP A0A369AIV8
B	-17	SER	-	expression tag	UNP A0A369AIV8
B	-16	SER	-	expression tag	UNP A0A369AIV8
B	-15	GLY	-	expression tag	UNP A0A369AIV8
B	-14	VAL	-	expression tag	UNP A0A369AIV8
B	-13	ASP	-	expression tag	UNP A0A369AIV8
B	-12	LEU	-	expression tag	UNP A0A369AIV8
B	-11	GLY	-	expression tag	UNP A0A369AIV8
B	-10	THR	-	expression tag	UNP A0A369AIV8
B	-9	GLU	-	expression tag	UNP A0A369AIV8
B	-8	ASN	-	expression tag	UNP A0A369AIV8
B	-7	LEU	-	expression tag	UNP A0A369AIV8
B	-6	TYR	-	expression tag	UNP A0A369AIV8
B	-5	PHE	-	expression tag	UNP A0A369AIV8
B	-4	GLN	-	expression tag	UNP A0A369AIV8
B	-3	SER	-	expression tag	UNP A0A369AIV8
B	-2	ASN	-	expression tag	UNP A0A369AIV8
B	-1	ALA	-	expression tag	UNP A0A369AIV8
B	0	MET	-	expression tag	UNP A0A369AIV8
B	422	GLU	-	cloning artifact	UNP A0A369AIV8
C	-24	MET	-	initiating methionine	UNP A0A369AIV8
C	-23	HIS	-	expression tag	UNP A0A369AIV8
C	-22	HIS	-	expression tag	UNP A0A369AIV8
C	-21	HIS	-	expression tag	UNP A0A369AIV8
C	-20	HIS	-	expression tag	UNP A0A369AIV8
C	-19	HIS	-	expression tag	UNP A0A369AIV8
C	-18	HIS	-	expression tag	UNP A0A369AIV8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP A0A369AIV8
C	-16	SER	-	expression tag	UNP A0A369AIV8
C	-15	GLY	-	expression tag	UNP A0A369AIV8
C	-14	VAL	-	expression tag	UNP A0A369AIV8
C	-13	ASP	-	expression tag	UNP A0A369AIV8
C	-12	LEU	-	expression tag	UNP A0A369AIV8
C	-11	GLY	-	expression tag	UNP A0A369AIV8
C	-10	THR	-	expression tag	UNP A0A369AIV8
C	-9	GLU	-	expression tag	UNP A0A369AIV8
C	-8	ASN	-	expression tag	UNP A0A369AIV8
C	-7	LEU	-	expression tag	UNP A0A369AIV8
C	-6	TYR	-	expression tag	UNP A0A369AIV8
C	-5	PHE	-	expression tag	UNP A0A369AIV8
C	-4	GLN	-	expression tag	UNP A0A369AIV8
C	-3	SER	-	expression tag	UNP A0A369AIV8
C	-2	ASN	-	expression tag	UNP A0A369AIV8
C	-1	ALA	-	expression tag	UNP A0A369AIV8
C	0	MET	-	expression tag	UNP A0A369AIV8
C	422	GLU	-	cloning artifact	UNP A0A369AIV8
D	-24	MET	-	initiating methionine	UNP A0A369AIV8
D	-23	HIS	-	expression tag	UNP A0A369AIV8
D	-22	HIS	-	expression tag	UNP A0A369AIV8
D	-21	HIS	-	expression tag	UNP A0A369AIV8
D	-20	HIS	-	expression tag	UNP A0A369AIV8
D	-19	HIS	-	expression tag	UNP A0A369AIV8
D	-18	HIS	-	expression tag	UNP A0A369AIV8
D	-17	SER	-	expression tag	UNP A0A369AIV8
D	-16	SER	-	expression tag	UNP A0A369AIV8
D	-15	GLY	-	expression tag	UNP A0A369AIV8
D	-14	VAL	-	expression tag	UNP A0A369AIV8
D	-13	ASP	-	expression tag	UNP A0A369AIV8
D	-12	LEU	-	expression tag	UNP A0A369AIV8
D	-11	GLY	-	expression tag	UNP A0A369AIV8
D	-10	THR	-	expression tag	UNP A0A369AIV8
D	-9	GLU	-	expression tag	UNP A0A369AIV8
D	-8	ASN	-	expression tag	UNP A0A369AIV8
D	-7	LEU	-	expression tag	UNP A0A369AIV8
D	-6	TYR	-	expression tag	UNP A0A369AIV8
D	-5	PHE	-	expression tag	UNP A0A369AIV8
D	-4	GLN	-	expression tag	UNP A0A369AIV8
D	-3	SER	-	expression tag	UNP A0A369AIV8
D	-2	ASN	-	expression tag	UNP A0A369AIV8

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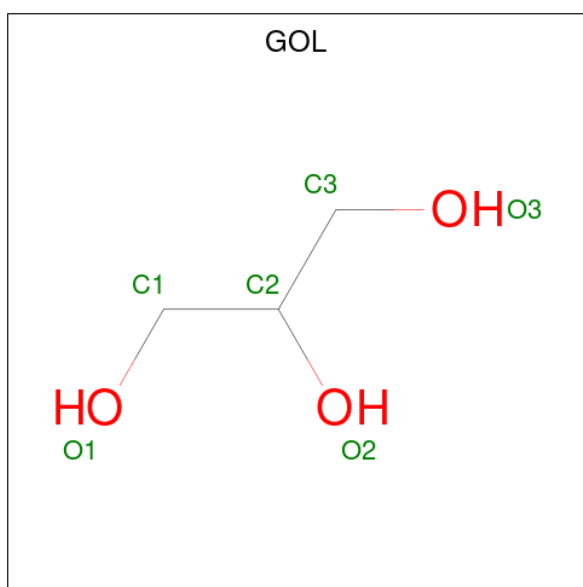
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ALA	-	expression tag	UNP A0A369AIV8
D	0	MET	-	expression tag	UNP A0A369AIV8
D	422	GLU	-	cloning artifact	UNP A0A369AIV8
E	-24	MET	-	initiating methionine	UNP A0A369AIV8
E	-23	HIS	-	expression tag	UNP A0A369AIV8
E	-22	HIS	-	expression tag	UNP A0A369AIV8
E	-21	HIS	-	expression tag	UNP A0A369AIV8
E	-20	HIS	-	expression tag	UNP A0A369AIV8
E	-19	HIS	-	expression tag	UNP A0A369AIV8
E	-18	HIS	-	expression tag	UNP A0A369AIV8
E	-17	SER	-	expression tag	UNP A0A369AIV8
E	-16	SER	-	expression tag	UNP A0A369AIV8
E	-15	GLY	-	expression tag	UNP A0A369AIV8
E	-14	VAL	-	expression tag	UNP A0A369AIV8
E	-13	ASP	-	expression tag	UNP A0A369AIV8
E	-12	LEU	-	expression tag	UNP A0A369AIV8
E	-11	GLY	-	expression tag	UNP A0A369AIV8
E	-10	THR	-	expression tag	UNP A0A369AIV8
E	-9	GLU	-	expression tag	UNP A0A369AIV8
E	-8	ASN	-	expression tag	UNP A0A369AIV8
E	-7	LEU	-	expression tag	UNP A0A369AIV8
E	-6	TYR	-	expression tag	UNP A0A369AIV8
E	-5	PHE	-	expression tag	UNP A0A369AIV8
E	-4	GLN	-	expression tag	UNP A0A369AIV8
E	-3	SER	-	expression tag	UNP A0A369AIV8
E	-2	ASN	-	expression tag	UNP A0A369AIV8
E	-1	ALA	-	expression tag	UNP A0A369AIV8
E	0	MET	-	expression tag	UNP A0A369AIV8
E	422	GLU	-	cloning artifact	UNP A0A369AIV8
F	-24	MET	-	initiating methionine	UNP A0A369AIV8
F	-23	HIS	-	expression tag	UNP A0A369AIV8
F	-22	HIS	-	expression tag	UNP A0A369AIV8
F	-21	HIS	-	expression tag	UNP A0A369AIV8
F	-20	HIS	-	expression tag	UNP A0A369AIV8
F	-19	HIS	-	expression tag	UNP A0A369AIV8
F	-18	HIS	-	expression tag	UNP A0A369AIV8
F	-17	SER	-	expression tag	UNP A0A369AIV8
F	-16	SER	-	expression tag	UNP A0A369AIV8
F	-15	GLY	-	expression tag	UNP A0A369AIV8
F	-14	VAL	-	expression tag	UNP A0A369AIV8
F	-13	ASP	-	expression tag	UNP A0A369AIV8
F	-12	LEU	-	expression tag	UNP A0A369AIV8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	GLY	-	expression tag	UNP A0A369AIV8
F	-10	THR	-	expression tag	UNP A0A369AIV8
F	-9	GLU	-	expression tag	UNP A0A369AIV8
F	-8	ASN	-	expression tag	UNP A0A369AIV8
F	-7	LEU	-	expression tag	UNP A0A369AIV8
F	-6	TYR	-	expression tag	UNP A0A369AIV8
F	-5	PHE	-	expression tag	UNP A0A369AIV8
F	-4	GLN	-	expression tag	UNP A0A369AIV8
F	-3	SER	-	expression tag	UNP A0A369AIV8
F	-2	ASN	-	expression tag	UNP A0A369AIV8
F	-1	ALA	-	expression tag	UNP A0A369AIV8
F	0	MET	-	expression tag	UNP A0A369AIV8
F	422	GLU	-	cloning artifact	UNP A0A369AIV8

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



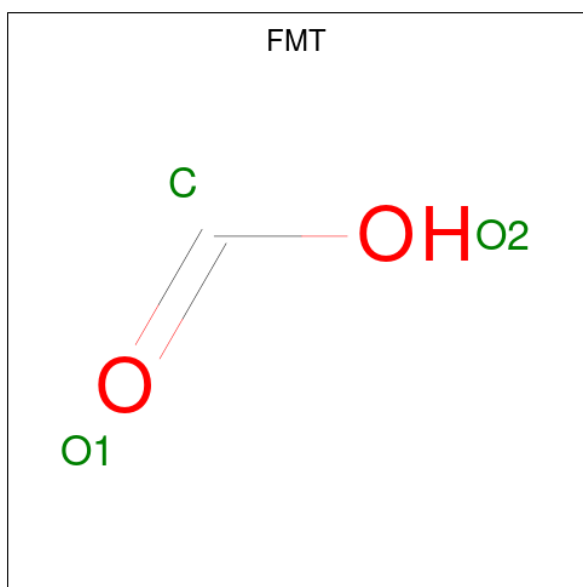
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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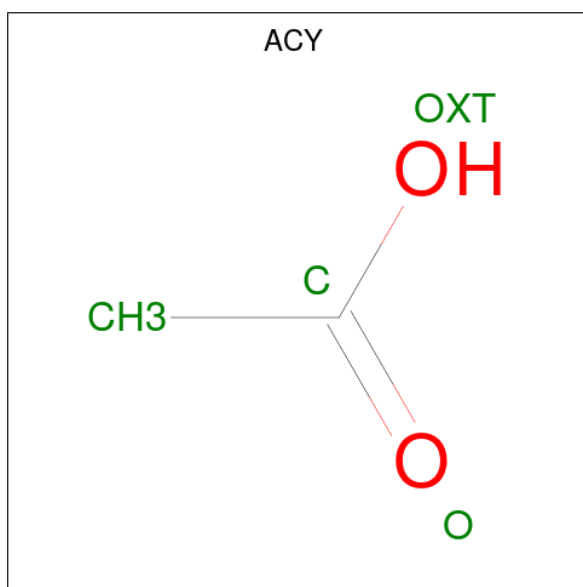
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	1
			12	6	6		
2	C	1	Total	C	O	0	1
			12	6	6		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

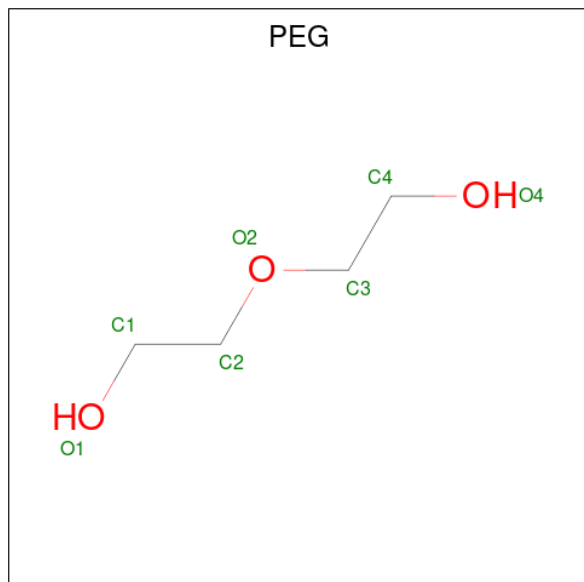


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	B	1	Total Na 1 1	0	0
6	C	1	Total Na 1 1	0	0
6	D	1	Total Na 1 1	0	0
6	E	1	Total Na 1 1	0	0
6	F	1	Total Na 1 1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0
7	F	1	Total C O 7 4 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	291	Total O 291 291	0	0

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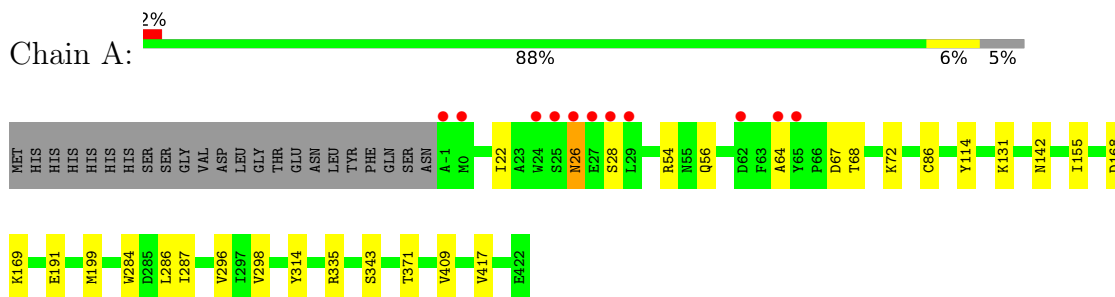
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	302	Total 302	O 302	0	0
8	C	279	Total 279	O 279	0	0
8	D	258	Total 258	O 258	0	0
8	E	220	Total 220	O 220	0	0
8	F	280	Total 280	O 280	0	0

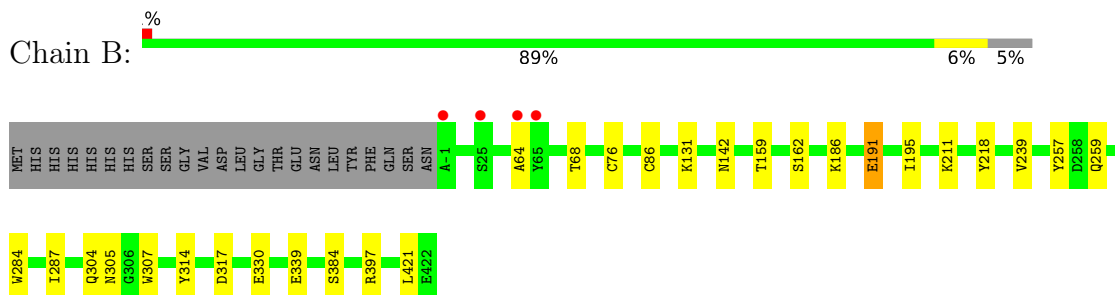
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

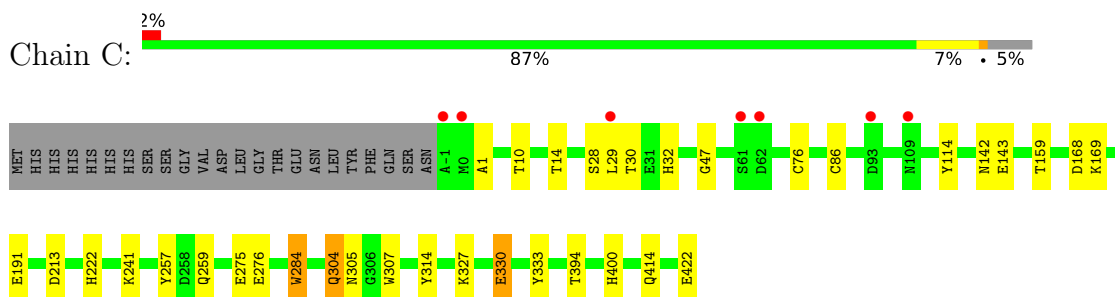
- Molecule 1: Glucuronarabinoxylan endo-1,4-beta-xylanase



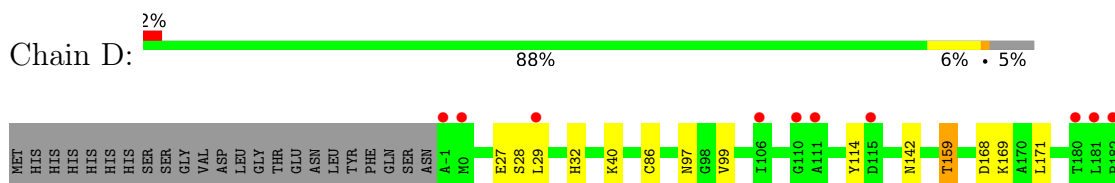
- Molecule 1: Glucuronarabinoxylan endo-1,4-beta-xylanase

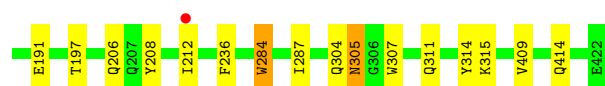


- Molecule 1: Glucuronarabinoxylan endo-1,4-beta-xylanase

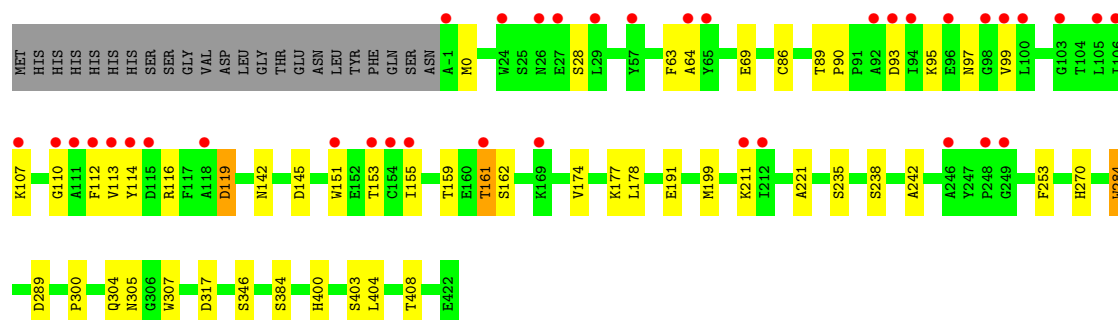
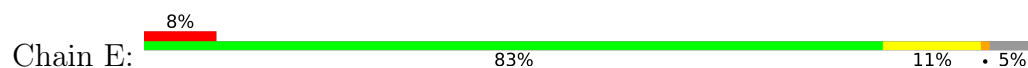


- Molecule 1: Glucuronarabinoxylan endo-1,4-beta-xylanase

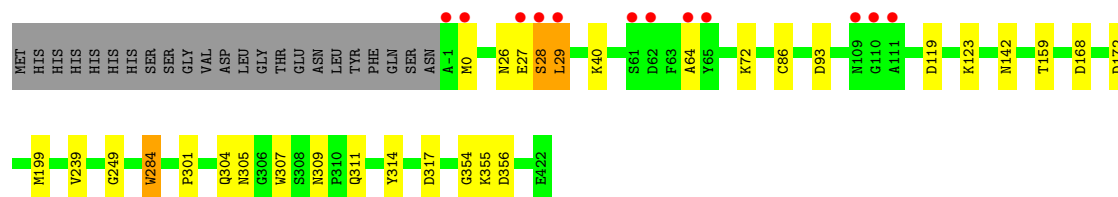
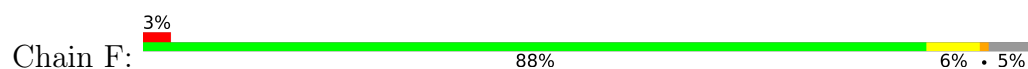




- Molecule 1: Glucuronoarabinoxylan endo-1,4-beta-xyranase



- Molecule 1: Glucuronoarabinoxylan endo-1,4-beta-xyranase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.31Å 133.39Å 137.70Å 90.00° 101.54° 90.00°	Depositor
Resolution (Å)	48.95 – 1.92 48.95 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.95-1.92) 99.0 (48.95-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.169 , 0.205 0.177 , 0.212	Depositor DCC
R_{free} test set	11805 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22256	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NA, FMT, EDO, GOL, ACY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/3489	1.03	2/4760 (0.0%)
1	B	0.63	0/3489	1.00	2/4759 (0.0%)
1	C	0.62	0/3488	1.00	4/4759 (0.1%)
1	D	0.61	0/3502	1.01	5/4776 (0.1%)
1	E	0.61	0/3484	1.03	5/4753 (0.1%)
1	F	0.61	0/3481	1.02	5/4748 (0.1%)
All	All	0.62	0/20933	1.01	23/28555 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	408	THR	CA-CB-OG1	-7.34	98.58	109.60
1	E	93	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	371	THR	CA-CB-OG1	-5.97	100.64	109.60
1	F	93	ASP	CA-CB-CG	5.94	118.54	112.60
1	D	311	GLN	CB-CA-C	-5.90	97.66	109.99
1	B	317	ASP	CA-CB-CG	5.77	118.37	112.60
1	D	159	THR	CA-CB-OG1	-5.72	101.01	109.60
1	A	168	ASP	CA-CB-CG	5.72	118.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	10	THR	CA-CB-OG1	-5.70	101.05	109.60
1	E	300	PRO	CB-CA-C	5.58	117.73	110.92
1	F	172	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	197	THR	CA-CB-OG1	-5.41	101.49	109.60
1	C	213	ASP	CA-CB-CG	5.38	117.98	112.60
1	D	168	ASP	CA-CB-CG	5.38	117.98	112.60
1	F	317	ASP	CA-CB-CG	5.37	117.97	112.60
1	E	317	ASP	CA-CB-CG	5.35	117.95	112.60
1	F	29	LEU	N-CA-CB	-5.26	102.92	110.65
1	C	14	THR	CA-CB-OG1	-5.21	101.79	109.60
1	E	161	THR	CA-CB-OG1	-5.12	101.92	109.60
1	F	168	ASP	CA-CB-CG	5.04	117.64	112.60
1	D	236	PHE	CA-CB-CG	5.02	118.82	113.80
1	C	394	THR	CA-CB-OG1	-5.01	102.08	109.60
1	B	191	GLU	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	ARG	Sidechain
1	A	54	ARG	Sidechain
1	A	64	ALA	Peptide
1	B	64	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3391	0	3240	22	0
1	B	3394	0	3235	16	0
1	C	3387	0	3236	20	0
1	D	3404	0	3256	19	0
1	E	3388	0	3227	37	0
1	F	3383	0	3229	25	0
2	A	24	0	32	0	0
2	B	30	0	40	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	64	2	0
2	D	18	0	24	1	0
2	E	18	0	24	9	0
2	F	6	0	8	0	0
3	A	3	0	1	0	0
3	B	3	0	2	0	0
3	C	6	0	4	0	0
3	D	12	0	6	0	0
3	E	6	0	4	0	0
3	F	6	0	4	0	0
4	A	8	0	6	1	0
4	C	8	0	6	3	0
4	E	4	0	3	1	0
4	F	4	0	3	0	0
5	A	4	0	6	0	0
5	B	16	0	24	2	0
5	C	4	0	6	1	0
5	D	4	0	6	3	0
5	E	4	0	6	0	0
5	F	16	0	24	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	B	7	0	10	0	0
7	D	7	0	10	0	0
7	F	7	0	10	0	0
8	A	291	0	0	2	1
8	B	302	0	0	4	1
8	C	279	0	0	7	0
8	D	258	0	0	4	1
8	E	220	0	0	5	1
8	F	280	0	0	6	0
All	All	22256	0	19756	143	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287[B]:ILE:HD11	1:A:298[B]:VAL:CG1	1.86	1.05
1:A:287[B]:ILE:HD11	1:A:298[B]:VAL:HG11	1.06	1.03
2:D:507:GOL:O1	8:D:601:HOH:O	1.77	1.01
1:D:40[A]:LYS:HE2	8:D:735:HOH:O	1.60	1.00
1:C:76[B]:CYS:SG	8:D:657:HOH:O	2.20	0.98
1:A:287[B]:ILE:CD1	1:A:298[B]:VAL:HG11	1.94	0.97
5:B:511:EDO:H11	1:D:315:LYS:HG3	1.52	0.91
1:D:208:TYR:O	1:D:212:ILE:HG12	1.73	0.88
1:E:113[B]:VAL:HG12	1:E:113[B]:VAL:O	1.73	0.86
1:E:235:SER:O	2:E:502:GOL:H2	1.75	0.86
1:E:86[B]:CYS:SG	1:E:142:ASN:HB2	2.18	0.83
1:A:287[B]:ILE:CD1	1:A:298[B]:VAL:CG1	2.58	0.79
1:A:287[B]:ILE:HG13	1:A:298[B]:VAL:HG13	1.65	0.79
1:C:1:ALA:O	5:C:511:EDO:H22	1.85	0.75
1:F:29:LEU:O	8:F:601:HOH:O	2.05	0.75
1:D:86[B]:CYS:SG	1:D:191:GLU:OE1	2.48	0.72
1:E:145:ASP:O	8:E:602:HOH:O	2.05	0.72
1:B:86[B]:CYS:SG	1:B:191:GLU:OE2	2.43	0.70
2:B:501:GOL:O1	8:B:601:HOH:O	2.12	0.68
1:D:40[A]:LYS:HE3	8:D:696:HOH:O	1.94	0.68
1:E:113[B]:VAL:O	1:E:113[B]:VAL:CG1	2.42	0.67
1:C:330[B]:GLU:OE1	8:C:602:HOH:O	2.13	0.66
1:B:330[B]:GLU:OE1	8:B:602:HOH:O	2.15	0.65
1:B:314:TYR:HB2	1:F:305[B]:ASN:HB3	1.77	0.65
1:E:113[B]:VAL:CG1	1:E:116:ARG:HB2	2.27	0.64
1:A:287[B]:ILE:CG1	1:A:298[B]:VAL:HG13	2.28	0.64
1:E:238:SER:OG	2:E:502:GOL:H12	1.99	0.63
1:C:29:LEU:C	8:C:606:HOH:O	2.44	0.60
1:F:239:VAL:HG23	8:F:602:HOH:O	2.01	0.60
1:F:64:ALA:HA	8:F:778:HOH:O	2.02	0.59
1:E:242:ALA:C	2:E:506:GOL:O2	2.46	0.58
1:A:314:TYR:HB2	1:C:305[B]:ASN:HB3	1.83	0.58
1:E:238:SER:OG	2:E:502:GOL:C1	2.52	0.58
1:E:400:HIS:HB3	1:F:40:LYS:HD3	1.86	0.58
1:A:287[B]:ILE:CG1	1:A:298[B]:VAL:CG1	2.81	0.57
1:C:330[B]:GLU:HG2	1:C:333:TYR:CE1	2.40	0.56
1:E:161:THR:HG22	1:E:162:SER:H	1.70	0.56
1:F:86[B]:CYS:SG	1:F:142:ASN:HB2	2.46	0.56
1:A:287[A]:ILE:C	1:A:287[A]:ILE:HD12	2.31	0.55
1:F:304[C]:GLN:O	1:F:304[C]:GLN:CD	2.49	0.55
1:E:90:PRO:HD2	1:E:95:LYS:HD3	1.89	0.55
2:E:506:GOL:C3	8:E:634:HOH:O	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:THR:HG22	1:C:168:ASP:OD2	2.09	0.54
1:A:28:SER:OG	1:A:298[A]:VAL:HG21	2.09	0.53
4:C:504:ACY:CH3	8:C:858:HOH:O	2.56	0.53
1:E:155:ILE:HD12	1:E:199:MET:HE1	1.91	0.53
1:D:29[A]:LEU:HD11	1:D:287:ILE:CD1	2.39	0.52
1:B:257:TYR:CZ	1:B:259:GLN:HB2	2.44	0.52
1:A:86[B]:CYS:SG	1:A:142:ASN:HB2	2.49	0.52
1:D:206:GLN:HE21	5:D:505:EDO:C2	2.23	0.52
5:B:511:EDO:H21	8:B:630:HOH:O	2.10	0.52
1:E:89:THR:OG1	1:E:90:PRO:HD2	2.09	0.52
1:E:159:THR:HG23	1:E:211:LYS:HG2	1.93	0.50
1:E:161:THR:HG22	1:E:162:SER:N	2.25	0.50
1:B:195:ILE:HD12	1:B:239:VAL:HG13	1.93	0.50
1:C:30:THR:N	8:C:606:HOH:O	2.43	0.50
1:C:304:GLN:HA	1:C:307:TRP:CD2	2.46	0.49
1:C:114:TYR:CE2	1:C:169:LYS:HE3	2.48	0.49
1:D:86[B]:CYS:SG	1:D:142:ASN:HB2	2.52	0.49
1:B:287:ILE:C	1:B:287:ILE:HD12	2.38	0.48
1:D:28[A]:SER:O	1:D:32:HIS:HB2	2.12	0.48
4:C:507:ACY:H1	8:C:795:HOH:O	2.13	0.48
1:F:27:GLU:C	1:F:29:LEU:H	2.21	0.48
1:F:27:GLU:C	1:F:29:LEU:N	2.71	0.48
1:E:384[B]:SER:O	1:E:403:SER:HA	2.14	0.48
4:C:507:ACY:CH3	8:C:795:HOH:O	2.61	0.47
1:D:171:LEU:CD2	1:D:212:ILE:HG23	2.43	0.47
2:E:506:GOL:H31	8:E:634:HOH:O	2.15	0.47
1:E:235:SER:O	2:E:502:GOL:C2	2.57	0.47
1:F:304[C]:GLN:CD	1:F:304[C]:GLN:C	2.82	0.47
1:D:27:GLU:O	1:D:28[A]:SER:C	2.57	0.47
1:F:199:MET:SD	8:F:852:HOH:O	2.61	0.47
1:C:86[B]:CYS:SG	1:C:142:ASN:HB2	2.55	0.47
1:C:257:TYR:CZ	1:C:259:GLN:HB2	2.49	0.47
1:F:309:ASN:OD1	1:F:311:GLN:HG2	2.15	0.47
1:E:174:VAL:O	1:E:178:LEU:HG	2.14	0.47
1:A:26[A]:ASN:ND2	1:A:28:SER:HB3	2.29	0.46
1:D:206:GLN:HG2	5:D:505:EDO:H22	1.97	0.46
4:E:504:ACY:H3	8:E:758:HOH:O	2.13	0.46
1:E:112:PHE:HB2	1:E:114[B]:TYR:CE2	2.51	0.46
1:F:239:VAL:N	8:F:602:HOH:O	2.24	0.46
1:B:384:SER:HB3	1:B:421:LEU:HD23	1.99	0.45
1:C:314:TYR:HB2	1:E:305:ASN:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ASN:HB3	1:F:314:TYR:HB2	1.98	0.45
1:B:68:THR:HG21	1:B:131:LYS:HB3	1.98	0.45
1:C:86[B]:CYS:SG	1:C:191:GLU:OE2	2.58	0.45
1:F:305[A]:ASN:ND2	8:F:606:HOH:O	2.44	0.45
1:A:114:TYR:CE2	1:A:169:LYS:HD2	2.52	0.45
1:B:397:ARG:NH2	1:F:304[B]:GLN:OE1	2.50	0.45
1:D:206:GLN:HG2	5:D:505:EDO:C2	2.46	0.45
2:C:503:GOL:C1	8:C:819:HOH:O	2.65	0.45
1:E:119:ASP:OD2	1:E:177:LYS:HE2	2.16	0.45
1:C:28:SER:O	1:C:32:HIS:HB2	2.17	0.44
1:C:400:HIS:HB3	1:D:40[A]:LYS:HD2	1.99	0.44
1:D:304:GLN:HA	1:D:307:TRP:CD2	2.53	0.44
1:B:159:THR:CG2	1:B:211:LYS:HD2	2.47	0.44
1:C:143:GLU:OE1	2:C:502:GOL:H31	2.18	0.44
1:A:86[B]:CYS:SG	1:A:191:GLU:OE1	2.64	0.44
1:B:305[B]:ASN:HB3	1:D:314:TYR:HB2	1.99	0.44
1:A:155:ILE:HD12	1:A:199:MET:HE1	2.00	0.44
1:B:86[B]:CYS:SG	1:B:142:ASN:HB2	2.58	0.44
1:E:107:LYS:HD3	1:E:110:GLY:C	2.43	0.44
1:E:384[B]:SER:OG	1:E:404:LEU:HB2	2.18	0.43
1:F:26:ASN:OD1	1:F:28:SER:CB	2.67	0.43
8:A:680:HOH:O	1:B:76[B]:CYS:SG	2.61	0.43
1:E:289:ASP:OD1	1:E:289:ASP:C	2.62	0.43
1:C:222:HIS:NE2	1:C:276:GLU:OE2	2.46	0.43
1:F:249:GLY:HA3	5:F:506:EDO:H22	2.00	0.43
1:A:409:VAL:HG21	1:A:417:VAL:HG11	2.01	0.43
1:E:63:PHE:O	1:E:64:ALA:HB3	2.19	0.43
1:F:356:ASP:OD1	1:F:356:ASP:N	2.43	0.43
1:B:339:GLU:OE1	2:B:502:GOL:H12	2.19	0.42
4:A:505:ACY:H1	8:A:858:HOH:O	2.19	0.42
1:A:56[B]:GLN:NE2	1:A:67:ASP:OD2	2.53	0.42
1:F:354:GLY:O	1:F:355:LYS:HB2	2.20	0.42
1:B:304:GLN:HA	1:B:307:TRP:CD2	2.55	0.42
2:B:502:GOL:O2	8:B:603:HOH:O	2.20	0.42
1:E:242:ALA:HB1	2:E:506:GOL:H12	2.01	0.42
1:A:68:THR:O	1:A:72:LYS:HG2	2.20	0.42
1:E:304[B]:GLN:HA	1:E:307:TRP:CE2	2.55	0.42
1:F:304[A]:GLN:HA	1:F:307:TRP:CD2	2.54	0.42
1:C:47:GLY:HA3	1:C:327:LYS:HA	2.02	0.42
1:D:114:TYR:CE2	1:D:169:LYS:HD2	2.55	0.41
1:E:238:SER:OG	2:E:502:GOL:H11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:LYS:HE3	1:C:275:GLU:OE1	2.21	0.41
1:F:28:SER:HA	1:F:301:PRO:HG3	2.02	0.41
1:E:113[B]:VAL:HG13	1:E:116:ARG:HB2	2.02	0.41
1:A:22:ILE:HD11	1:A:286:LEU:HD23	2.03	0.41
1:E:0:MET:HE3	8:E:802:HOH:O	2.21	0.41
1:A:68:THR:HG22	1:A:131:LYS:HB3	2.03	0.41
1:E:270:HIS:CE1	1:E:346:SER:HB3	2.56	0.41
1:F:304[A]:GLN:HA	1:F:307:TRP:CE2	2.56	0.41
1:E:97:ASN:HB2	1:E:99:VAL:HG23	2.03	0.41
1:E:151:TRP:O	1:E:153:THR:HG23	2.20	0.40
1:A:287[A]:ILE:HD12	1:A:287[A]:ILE:O	2.20	0.40
1:E:221:ALA:HA	1:E:253:PHE:O	2.20	0.40
1:E:304[A]:GLN:HA	1:E:307:TRP:CD2	2.56	0.40
1:B:186:LYS:HB3	1:B:218:TYR:CB	2.50	0.40
1:F:26:ASN:OD1	1:F:28:SER:HB2	2.22	0.40
1:A:287[B]:ILE:HA	1:A:296:VAL:O	2.22	0.40
1:D:97:ASN:HB2	1:D:99:VAL:HG23	2.04	0.40
1:E:86[B]:CYS:SG	1:E:191:GLU:OE1	2.65	0.40
1:F:119:ASP:OD2	1:F:123[B]:LYS:NZ	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:847:HOH:O	8:D:748:HOH:O[2_455]	2.13	0.07
8:A:827:HOH:O	8:E:710:HOH:O[2_446]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	432/447 (97%)	422 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	432/447 (97%)	420 (97%)	12 (3%)	0	100	100
1	C	432/447 (97%)	420 (97%)	11 (2%)	1 (0%)	43	34
1	D	434/447 (97%)	416 (96%)	17 (4%)	1 (0%)	43	34
1	E	431/447 (96%)	409 (95%)	21 (5%)	1 (0%)	43	34
1	F	430/447 (96%)	412 (96%)	16 (4%)	2 (0%)	24	14
All	All	2591/2682 (97%)	2499 (96%)	87 (3%)	5 (0%)	43	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	28	SER
1	C	284	TRP
1	D	284	TRP
1	E	284	TRP
1	F	284	TRP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/381 (97%)	366 (99%)	4 (1%)	65	60
1	B	370/381 (97%)	368 (100%)	2 (0%)	81	80
1	C	370/381 (97%)	364 (98%)	6 (2%)	55	44
1	D	372/381 (98%)	367 (99%)	5 (1%)	61	53
1	E	369/381 (97%)	365 (99%)	4 (1%)	65	60
1	F	368/381 (97%)	364 (99%)	4 (1%)	65	60
All	All	2219/2286 (97%)	2194 (99%)	25 (1%)	65	60

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26[A]	ASN

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Mol	Chain	Res	Type
1	A	26[B]	ASN
1	A	284	TRP
1	A	343	SER
1	B	162	SER
1	B	284	TRP
1	C	284	TRP
1	C	304	GLN
1	C	330[A]	GLU
1	C	330[B]	GLU
1	C	414	GLN
1	C	422	GLU
1	D	159	THR
1	D	284	TRP
1	D	305	ASN
1	D	409	VAL
1	D	414	GLN
1	E	28	SER
1	E	69	GLU
1	E	119	ASP
1	E	284	TRP
1	F	0	MET
1	F	72	LYS
1	F	159	THR
1	F	284	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	311	GLN
1	B	267	GLN
1	B	311	GLN
1	C	9	ASN
1	C	56	GLN
1	C	141	GLN
1	C	375	ASN
1	C	377	ASN
1	D	267	GLN
1	D	377	ASN
1	E	56	GLN
1	E	231	ASN
1	E	311	GLN

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Mol	Chain	Res	Type
1	E	377	ASN
1	F	56	GLN
1	F	80	ASN
1	F	97	ASN
1	F	126	ASN
1	F	405	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 6 are monoatomic - leaving 57 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	F	504	-	3,3,3	0.17	0	2,2,2	0.32	0
5	EDO	E	505	-	3,3,3	0.07	0	2,2,2	0.04	0
2	GOL	F	502	-	5,5,5	0.14	0	5,5,5	0.46	0
2	GOL	C	509[A]	-	5,5,5	0.15	0	5,5,5	0.38	0
3	FMT	E	503	-	2,2,2	1.14	0	1,1,1	0.18	0
2	GOL	B	504	-	5,5,5	0.22	0	5,5,5	0.54	0
2	GOL	B	502	-	5,5,5	0.14	0	5,5,5	0.48	0
7	PEG	B	506	-	6,6,6	0.09	0	5,5,5	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	F	503	-	3,3,3	0.52	0	2,2,2	0.15	0
2	GOL	B	507	-	5,5,5	0.09	0	5,5,5	0.26	0
5	EDO	B	505	-	3,3,3	0.17	0	2,2,2	0.06	0
2	GOL	B	503	-	5,5,5	0.11	0	5,5,5	0.33	0
2	GOL	D	501	-	5,5,5	0.16	0	5,5,5	0.48	0
4	ACY	E	504	-	3,3,3	0.81	0	3,3,3	1.26	0
3	FMT	E	507	-	2,2,2	1.53	1 (50%)	1,1,1	0.02	0
5	EDO	F	509	-	3,3,3	0.41	0	2,2,2	0.68	0
3	FMT	B	509	-	2,2,2	1.55	1 (50%)	1,1,1	0.07	0
2	GOL	C	508[B]	-	5,5,5	0.12	0	5,5,5	0.37	0
2	GOL	A	501	-	5,5,5	0.14	0	5,5,5	0.23	0
2	GOL	C	510	-	5,5,5	0.09	0	5,5,5	0.31	0
2	GOL	C	502	-	5,5,5	0.11	0	5,5,5	0.42	0
3	FMT	A	504	-	2,2,2	1.10	0	1,1,1	0.24	0
3	FMT	C	506	-	2,2,2	1.38	0	1,1,1	0.13	0
7	PEG	D	508	-	6,6,6	0.31	0	5,5,5	0.28	0
2	GOL	C	508[A]	-	5,5,5	0.11	0	5,5,5	0.29	0
5	EDO	C	511	-	3,3,3	0.25	0	2,2,2	0.59	0
2	GOL	B	501	-	5,5,5	0.25	0	5,5,5	0.78	0
5	EDO	A	506	-	3,3,3	0.22	0	2,2,2	0.36	0
7	PEG	F	507	-	6,6,6	0.16	0	5,5,5	0.10	0
3	FMT	D	503	-	2,2,2	0.87	0	1,1,1	0.28	0
4	ACY	A	508	-	3,3,3	1.17	0	3,3,3	0.69	0
5	EDO	B	508	-	3,3,3	0.20	0	2,2,2	0.23	0
4	ACY	F	505	-	3,3,3	1.25	0	3,3,3	0.63	0
5	EDO	B	510	-	3,3,3	0.42	0	2,2,2	0.45	0
3	FMT	D	502	-	2,2,2	1.24	0	1,1,1	0.14	0
2	GOL	D	504	-	5,5,5	0.17	0	5,5,5	0.43	0
4	ACY	C	504	-	3,3,3	0.87	0	3,3,3	1.08	0
5	EDO	F	506	-	3,3,3	0.31	0	2,2,2	0.42	0
3	FMT	D	506	6	2,2,2	1.12	0	1,1,1	0.20	0
2	GOL	A	503	-	5,5,5	0.12	0	5,5,5	0.32	0
3	FMT	D	509	-	2,2,2	1.21	0	1,1,1	0.11	0
2	GOL	C	505	-	5,5,5	0.08	0	5,5,5	0.37	0
2	GOL	A	502	-	5,5,5	0.14	0	5,5,5	0.44	0
2	GOL	C	503	-	5,5,5	0.13	0	5,5,5	0.32	0
4	ACY	A	505	-	3,3,3	1.08	0	3,3,3	1.00	0
4	ACY	C	507	-	3,3,3	0.79	0	3,3,3	1.55	1 (33%)
2	GOL	E	501	-	5,5,5	0.12	0	5,5,5	0.28	0
2	GOL	E	502	-	5,5,5	0.22	0	5,5,5	0.73	0
3	FMT	C	501	-	2,2,2	1.23	0	1,1,1	0.11	0
5	EDO	D	505	-	3,3,3	0.15	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	511	-	3,3,3	0.34	0	2,2,2	0.12	0
2	GOL	A	507	-	5,5,5	0.10	0	5,5,5	0.27	0
2	GOL	E	506	-	5,5,5	0.10	0	5,5,5	0.35	0
3	FMT	F	501	-	2,2,2	1.55	1 (50%)	1,1,1	0.11	0
2	GOL	D	507	-	5,5,5	0.13	0	5,5,5	0.44	0
2	GOL	C	509[B]	-	5,5,5	0.10	0	5,5,5	0.25	0
3	FMT	F	508	-	2,2,2	1.24	0	1,1,1	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	F	504	-	-	0/1/1/1	-
5	EDO	E	505	-	-	1/1/1/1	-
2	GOL	F	502	-	-	2/4/4/4	-
2	GOL	C	509[A]	-	-	1/4/4/4	-
2	GOL	B	504	-	-	4/4/4/4	-
2	GOL	B	502	-	-	4/4/4/4	-
7	PEG	B	506	-	-	1/4/4/4	-
5	EDO	F	503	-	-	0/1/1/1	-
2	GOL	B	507	-	-	0/4/4/4	-
5	EDO	B	505	-	-	0/1/1/1	-
2	GOL	B	503	-	-	0/4/4/4	-
2	GOL	D	501	-	-	0/4/4/4	-
5	EDO	F	509	-	-	1/1/1/1	-
2	GOL	C	508[B]	-	-	2/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-
2	GOL	C	510	-	-	1/4/4/4	-
2	GOL	C	502	-	-	1/4/4/4	-
7	PEG	D	508	-	-	3/4/4/4	-
2	GOL	C	508[A]	-	-	1/4/4/4	-
5	EDO	C	511	-	-	0/1/1/1	-
2	GOL	B	501	-	-	0/4/4/4	-
5	EDO	A	506	-	-	1/1/1/1	-
7	PEG	F	507	-	-	3/4/4/4	-
5	EDO	B	508	-	-	1/1/1/1	-
5	EDO	B	510	-	-	1/1/1/1	-
2	GOL	D	504	-	-	2/4/4/4	-
5	EDO	F	506	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	503	-	-	2/4/4/4	-
2	GOL	C	505	-	-	2/4/4/4	-
2	GOL	A	502	-	-	0/4/4/4	-
2	GOL	C	503	-	-	2/4/4/4	-
2	GOL	E	501	-	-	4/4/4/4	-
2	GOL	E	502	-	-	0/4/4/4	-
5	EDO	D	505	-	-	1/1/1/1	-
5	EDO	B	511	-	-	0/1/1/1	-
2	GOL	A	507	-	-	2/4/4/4	-
2	GOL	E	506	-	-	2/4/4/4	-
2	GOL	D	507	-	-	2/4/4/4	-
2	GOL	C	509[B]	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	FMT	O2-C	2.19	1.39	1.28
3	B	509	FMT	O2-C	2.18	1.39	1.28
3	E	507	FMT	O2-C	2.17	1.39	1.28

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	507	ACY	O-C-CH3	-2.11	113.89	122.53

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	A	503	GOL	O1-C1-C2-C3
2	A	507	GOL	C1-C2-C3-O3
2	B	502	GOL	O1-C1-C2-O2
2	B	502	GOL	O1-C1-C2-C3
2	B	502	GOL	C1-C2-C3-O3
2	B	504	GOL	O1-C1-C2-O2
2	B	504	GOL	C1-C2-C3-O3
2	C	503	GOL	O1-C1-C2-C3
2	C	505	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	C	508[B]	GOL	O1-C1-C2-C3
2	D	504	GOL	C1-C2-C3-O3
2	D	504	GOL	O2-C2-C3-O3
2	D	507	GOL	C1-C2-C3-O3
2	C	509[B]	GOL	O1-C1-C2-O2
2	B	504	GOL	O1-C1-C2-C3
2	C	502	GOL	O1-C1-C2-C3
2	C	505	GOL	C1-C2-C3-O3
2	C	508[A]	GOL	O1-C1-C2-C3
2	C	509[B]	GOL	O1-C1-C2-C3
2	E	501	GOL	C1-C2-C3-O3
2	E	506	GOL	O1-C1-C2-C3
7	F	507	PEG	O1-C1-C2-O2
2	A	501	GOL	O1-C1-C2-O2
2	A	503	GOL	O1-C1-C2-O2
2	C	503	GOL	O1-C1-C2-O2
2	C	508[B]	GOL	O1-C1-C2-O2
2	D	507	GOL	O2-C2-C3-O3
2	E	506	GOL	O1-C1-C2-O2
7	B	506	PEG	O1-C1-C2-O2
5	D	505	EDO	O1-C1-C2-O2
2	A	507	GOL	O2-C2-C3-O3
2	B	502	GOL	O2-C2-C3-O3
2	E	501	GOL	O2-C2-C3-O3
7	D	508	PEG	O2-C3-C4-O4
5	B	508	EDO	O1-C1-C2-O2
5	B	510	EDO	O1-C1-C2-O2
5	F	506	EDO	O1-C1-C2-O2
2	B	504	GOL	O2-C2-C3-O3
2	C	509[A]	GOL	O2-C2-C3-O3
2	E	501	GOL	O1-C1-C2-O2
7	D	508	PEG	O1-C1-C2-O2
7	D	508	PEG	C4-C3-O2-C2
5	A	506	EDO	O1-C1-C2-O2
7	F	507	PEG	O2-C3-C4-O4
2	F	502	GOL	O1-C1-C2-C3
2	F	502	GOL	O1-C1-C2-O2
2	E	501	GOL	O1-C1-C2-C3
7	F	507	PEG	C4-C3-O2-C2
5	F	509	EDO	O1-C1-C2-O2
2	C	510	GOL	O1-C1-C2-C3
5	E	505	EDO	O1-C1-C2-O2

There are no ring outliers.

15 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	GOL	2	0
4	E	504	ACY	1	0
2	C	502	GOL	1	0
5	C	511	EDO	1	0
2	B	501	GOL	1	0
4	C	504	ACY	1	0
5	F	506	EDO	1	0
2	C	503	GOL	1	0
4	A	505	ACY	1	0
4	C	507	ACY	2	0
2	E	502	GOL	5	0
5	D	505	EDO	3	0
5	B	511	EDO	2	0
2	E	506	GOL	4	0
2	D	507	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	424/447 (94%)	-0.22	11 (2%) 57 63	8, 22, 42, 73	10 (2%)
1	B	424/447 (94%)	-0.21	4 (0%) 81 86	10, 23, 44, 66	10 (2%)
1	C	424/447 (94%)	-0.11	7 (1%) 69 75	8, 25, 44, 72	10 (2%)
1	D	424/447 (94%)	0.05	11 (2%) 57 63	8, 27, 52, 72	12 (2%)
1	E	424/447 (94%)	0.37	37 (8%) 16 19	9, 30, 61, 85	9 (2%)
1	F	424/447 (94%)	-0.10	12 (2%) 55 61	6, 25, 46, 80	7 (1%)
All	All	2544/2682 (94%)	-0.04	82 (3%) 50 55	6, 25, 51, 85	58 (2%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26[A]	ASN	6.1
1	A	-1	ALA	4.7
1	E	29	LEU	4.4
1	C	-1	ALA	4.3
1	B	65	TYR	4.1
1	A	64	ALA	4.0
1	E	249	GLY	4.0
1	E	106	ILE	4.0
1	B	-1	ALA	3.9
1	B	64	ALA	3.7
1	F	110	GLY	3.7
1	E	110	GLY	3.6
1	E	113[A]	VAL	3.5
1	E	92	ALA	3.3
1	E	107	LYS	3.3
1	E	248	PRO	3.3
1	F	-1	ALA	3.2
1	A	28	SER	3.2
1	F	64	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	182	PRO	3.1
1	E	105	LEU	3.0
1	F	28	SER	2.9
1	A	27	GLU	2.9
1	A	0	MET	2.8
1	A	65	TYR	2.8
1	D	0	MET	2.8
1	E	111	ALA	2.8
1	A	29	LEU	2.8
1	C	0	MET	2.8
1	A	25	SER	2.7
1	E	24	TRP	2.7
1	E	211	LYS	2.7
1	D	29[A]	LEU	2.7
1	E	99	VAL	2.7
1	F	0	MET	2.6
1	E	93	ASP	2.6
1	E	103	GLY	2.6
1	F	27	GLU	2.6
1	D	110	GLY	2.6
1	E	-1	ALA	2.6
1	E	65	TYR	2.5
1	D	111	ALA	2.5
1	F	62	ASP	2.5
1	F	29	LEU	2.5
1	D	106	ILE	2.5
1	D	181	LEU	2.4
1	F	65	TYR	2.4
1	C	62	ASP	2.4
1	D	115	ASP	2.4
1	D	-1	ALA	2.4
1	E	161	THR	2.3
1	F	61	SER	2.3
1	E	98	GLY	2.3
1	A	62	ASP	2.3
1	E	112	PHE	2.2
1	D	212	ILE	2.2
1	E	27	GLU	2.2
1	F	111	ALA	2.2
1	E	155	ILE	2.2
1	B	25	SER	2.2
1	E	246	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	109	ASN	2.1
1	E	26	ASN	2.1
1	E	100	LEU	2.1
1	C	93	ASP	2.1
1	C	61	SER	2.1
1	E	94	ILE	2.1
1	E	114[A]	TYR	2.1
1	E	115	ASP	2.1
1	E	212	ILE	2.1
1	E	169	LYS	2.1
1	E	151	TRP	2.1
1	F	109	ASN	2.1
1	C	29	LEU	2.1
1	E	64	ALA	2.1
1	D	180	THR	2.0
1	E	153	THR	2.0
1	A	24	TRP	2.0
1	E	154	CYS	2.0
1	E	118	ALA	2.0
1	E	96	GLU	2.0
1	E	57	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ACY	A	505	4/4	0.72	0.23	55,60,63,65	0
5	EDO	B	505	4/4	0.72	0.22	58,58,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	PEG	D	508	7/7	0.73	0.23	65,77,89,91	0
5	EDO	C	511	4/4	0.76	0.25	76,80,81,81	0
2	GOL	B	503	6/6	0.76	0.25	54,69,71,73	0
2	GOL	E	506	6/6	0.78	0.23	63,68,69,78	0
2	GOL	C	509[B]	6/6	0.79	0.15	33,42,45,46	6
2	GOL	C	509[A]	6/6	0.79	0.15	33,41,42,43	6
7	PEG	B	506	7/7	0.81	0.18	71,75,77,78	0
2	GOL	A	507	6/6	0.81	0.18	67,73,75,76	0
2	GOL	C	505	6/6	0.82	0.16	45,57,59,62	0
4	ACY	F	505	4/4	0.82	0.17	51,57,58,59	0
2	GOL	E	501	6/6	0.83	0.19	63,66,68,71	0
2	GOL	C	510	6/6	0.83	0.17	47,58,59,62	0
4	ACY	A	508	4/4	0.84	0.19	51,59,64,65	0
2	GOL	E	502	6/6	0.84	0.14	36,46,53,54	0
2	GOL	D	501	6/6	0.85	0.17	55,57,59,60	0
2	GOL	B	507	6/6	0.86	0.14	51,53,56,59	0
5	EDO	B	510	4/4	0.86	0.15	45,47,49,49	0
4	ACY	C	507	4/4	0.86	0.17	30,46,46,48	0
4	ACY	E	504	4/4	0.86	0.16	30,42,48,56	0
2	GOL	B	504	6/6	0.86	0.17	37,56,60,61	0
2	GOL	C	502	6/6	0.87	0.15	51,51,54,56	0
2	GOL	B	501	6/6	0.87	0.17	42,45,48,56	0
2	GOL	D	504	6/6	0.87	0.14	32,49,55,62	0
3	FMT	C	501	3/3	0.87	0.18	39,39,41,43	0
3	FMT	D	503	3/3	0.87	0.15	49,49,52,56	0
2	GOL	C	508[A]	6/6	0.88	0.15	34,35,36,39	6
2	GOL	C	508[B]	6/6	0.88	0.15	39,41,45,45	6
5	EDO	E	505	4/4	0.88	0.16	54,64,65,68	0
2	GOL	F	502	6/6	0.88	0.17	52,57,58,61	0
3	FMT	A	504	3/3	0.88	0.22	55,55,61,66	0
2	GOL	D	507	6/6	0.89	0.12	46,55,56,60	0
5	EDO	F	504	4/4	0.89	0.19	41,45,46,51	0
3	FMT	C	506	3/3	0.89	0.13	37,37,40,43	0
5	EDO	A	506	4/4	0.89	0.17	46,47,49,53	0
7	PEG	F	507	7/7	0.89	0.14	51,58,66,67	0
3	FMT	F	501	3/3	0.90	0.15	33,33,37,38	0
2	GOL	C	503	6/6	0.90	0.13	34,46,50,58	0
5	EDO	F	506	4/4	0.90	0.14	44,47,49,51	0
5	EDO	F	509	4/4	0.90	0.10	24,31,36,42	0
2	GOL	A	502	6/6	0.90	0.13	42,43,47,51	0
2	GOL	A	503	6/6	0.90	0.13	35,53,60,60	0
3	FMT	E	503	3/3	0.90	0.24	47,47,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	501	6/6	0.91	0.11	29,30,36,44	0
2	GOL	B	502	6/6	0.91	0.12	32,49,53,57	0
3	FMT	D	502	3/3	0.92	0.12	39,39,49,50	0
5	EDO	B	511	4/4	0.92	0.12	26,28,31,33	0
5	EDO	F	503	4/4	0.92	0.11	28,29,30,35	0
5	EDO	D	505	4/4	0.93	0.10	41,44,46,48	0
5	EDO	B	508	4/4	0.93	0.12	42,45,46,46	0
3	FMT	E	507	3/3	0.93	0.11	29,29,32,35	0
3	FMT	D	506	3/3	0.94	0.11	42,42,44,51	0
4	ACY	C	504	4/4	0.94	0.12	32,35,38,48	0
3	FMT	F	508	3/3	0.94	0.09	26,26,37,45	0
3	FMT	D	509	3/3	0.94	0.08	35,35,35,35	0
6	NA	E	508	1/1	0.96	0.07	23,23,23,23	0
3	FMT	B	509	3/3	0.96	0.10	23,23,30,35	0
6	NA	C	512	1/1	0.97	0.08	19,19,19,19	0
6	NA	B	512	1/1	0.97	0.04	22,22,22,22	0
6	NA	F	510	1/1	0.97	0.05	18,18,18,18	0
6	NA	D	510	1/1	0.98	0.06	16,16,16,16	0
6	NA	A	509	1/1	0.99	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.